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Supplementary information

Selected ion flow tube mass spectrometry for targeted analysis of volatile organic compounds in human breath

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SUPPLEMENTARY INFORMATION

Supplementary Note 1: Literature Search. Literature search for breath studies conducted with SIFT-MS or all mass spectrometric techniques using titles and abstracts of research papers in English was performed via PubMed database on December 09, 2020.

For SIFT-MS breath studies the search criteria were ((sift-ms) OR (selected ion flow tube)) AND (breath) and identified 167 papers.

For all mass spectrometry approaches and breath the search criteria were (((((sift-ms[Title/Abstract]) OR (ptr-ms[Title/Abstract])) OR (gc-ms[Title/Abstract])) OR (sesi-ms[Title/Abstract])) OR (mass spectrometr*[Title/Abstract])) AND (breath[Title/Abstract]) and 1494 papers were identified.

Supplementary Table 1. Analytical methods developed with the SIFT-MS used to analyse groups of VOCs in human breath. For each of the four analytical methods compound name and formula, reagent ion, reaction rate, branching ratio and product ion name and formula are reported. In each of the analytical methods different product ions obtained with each of the three reagent ions are included, when possible. Hydrated forms can be produced given the natural moisture of breath. In grey, the product ions used for the quantification.

Method 1: ALCOHOLS						
Compound		Reagent Ion	Reaction Rate	Branching Ratio	Product Ion	
Acetone	C_3H_6O	H_3O^+	3.90E-09	100	59	$C_3H_7O^+$
		H_3O^+	3.90E-09	*hydrated*	77	$(CH_3)2CO.H^+.H_2O$
		NO^+	1.20E-09	100	88	$NO^+.C_3H_6O$
Isoprene	C_5H_8	H_3O^+	2.00E-09	100	69	$C_5H_8.H^+$
		NO^+	1.70E-09	100	68	$C_5H_8^+$
Methanol	CH_3OH	H_3O^+	2.70E-09	100	33	CH_5O^+
		H_3O^+	2.70E-09	*hydrated*	51	$CH_3OH_2^+.H_2O$
Ethanol	C_2H_5OH	H_3O^+	2.70E-09	100	47	$C_2H_7O^+$
		NO^+	1.20E-09	100	45	$C_2H_5O^+$
		NO^+	1.20E-09	*hydrated*	63	$C_2H_5O^+.H_2O$
1-butanol	$C_4H_{10}O$	H_3O^+	2.80E-09	95	57	$C_4H_9^+$
		NO^+	2.20E-09	95	73	$C_4H_9O^+$
		O_2^+	2.50E-09	80	56	$C_4H_8^+$
1-pentanol	$C_5H_{12}O$	H_3O^+	2.80E-09	100	71	$C_5H_{11}^+$
		NO^+	2.50E-09	85	87	$C_5H_{11}O^+$
		O_2^+	2.80E-09	45	70	$C_5H_{10}^+$

Method 2: ALDEHYDES						
Compound		Reagent Ion	Reaction Rate	Branching Ratio	Product Ion	
Acetone	C_3H_6O	H_3O^+	3.90E-09	100	59	$C_3H_7O^+$
		H_3O^+	3.90E-09	*hydrated*	77	$(CH_3)2CO.H^+.H_2O$
		NO^+	1.20E-09	100	88	$NO^+.C_3H_6O$
Acetaldehyde	C_2H_4O	H_3O^+	3.70E-09	100	45	$C_2H_5O^+$
		H_3O^+	3.70E-09	*hydrated*	63	$C_2H_5O^+.H_2O$
		NO^+	6.00E-10	100	43	CH_3CO^+
		NO^+	6.00E-10	*hydrated*	61	$CH_3CO^+.H_2O$
		NO^+	6.00E-10	*hydrated*	79	$CH_3CO^+.2H_2O$
		O_2^+	2.30E-09	45	43	$C_2H_3O^+$
		O_2^+	2.30E-09	55	44	$C_2H_4O^+$
Propanal	C_3H_6O	NO^+	2.50E-09	100	57	$C_3H_5O^+$
Butanal	C_4H_8O	NO^+	3.50E-09	100	71	$C_4H_7O^+$
		O_2^+	3.50E-09	65	44	$C_2H_4O^+$
		O_2^+	3.50E-09	35	72	$C_4H_8O^+$
Pentanal	$C_5H_{10}O$	H_3O^+	3.60E-09	65	87	$C_5H_{11}O^+$
		H_3O^+	3.60E-09	*hydrated*	105	$C_5H_{11}O^+.H_2O$
		H_3O^+	3.60E-09	*hydrated*	123	$C_5H_{11}O^+.2H_2O$
		NO^+	3.00E-09	100	85	$C_5H_9O^+$
Hexanal	$C_6H_{12}O$	H_3O^+	3.70E-09	50	83	$C_6H_{11}^+$
		H_3O^+	3.70E-09	50	101	$C_6H_{13}O^+$
		H_3O^+	3.70E-09	*hydrated*	119	$C_6H_{13}O^+.H_2O$
		H_3O^+	3.70E-09	*hydrated*	137	$C_6H_{13}O^+.2H_2O$
		NO^+	2.50E-09	100	99	$C_6H_{11}O^+$
Heptanal	$C_7H_{14}O$	H_3O^+	3.70E-09	80	115	$C_7H_{15}O^+$
		H_3O^+	3.70E-09	*hydrated*	133	$C_7H_{15}O^+.H_2O$
		NO^+	3.30E-09	100	113	$C_7H_{13}O^+$
		O_2^+	3.20E-09	22	96	$C_7H_{12}^+$
Octanal	$C_8H_{16}O$	H_3O^+	3.80E-09	85	129	$C_8H_{17}O^+$
		H_3O^+	3.80E-09	*hydrated*	147	$C_8H_{17}O^+.H_2O$
		H_3O^+	3.80E-09	*hydrated*	165	$C_8H_{17}O^+.2H_2O$
		NO^+	3.00E-09	100	127	$C_8H_{15}O^+$
		O_2^+	2.80E-09	45	84	$C_6H_{12}^+$
Nonanal	$C_9H_{18}O$	H_3O^+	2.50E-09	86	143	$C_9H_{19}O^+$
		NO^+	2.70E-09	100	141	$C_9H_{17}O^+$
Decanal	$C_{10}H_{20}O$	H_3O^+	3.90E-09	97	157	$C_{10}H_{21}O^+$
		H_3O^+	3.90E-09	*hydrated*	175	$C_{10}H_{21}O^+.H_2O$
		NO^+	3.30E-09	100	155	$C_{10}H_{19}O^+$

Method 3: PHENOLS AND ALKANES						
Compound		Reagent Ion	Reaction Rate	Branching Ratio	Product Ion	
Acetone	C_3H_6O	H_3O^+	3.90E-09	100	59	$C_3H_7O^+$
		H_3O^+	3.90E-09	*hydrated*	77	$(CH_3)2CO.H^+.H_2O$
		NO^+	1.20E-09	100	88	$NO^+.C_3H_6O$
Ammonia	NH_3	H_3O^+	2.60E-09	100	18	NH_4^+
		H_3O^+	2.60E-09	*hydrated*	36	$NH_4^+.H_2O$
		O_2^+	2.60E-09	100	17	NH_3^+
Phenol	C_6H_6O	H_3O^+	2.70E-09	100	95	$C_6H_7O^+$
		H_3O^+	2.70E-09	*hydrated*	113	$C_6H_7O^+.H_2O$
		NO^+	2.00E-09	100	94	$C_6H_6O^+$
		O_2^+	1.80E-09	100	94	$C_6H_6O^+$
P-cresol	C_7H_8O	H_3O^+	2.80E-09	100	109	$C_7H_9O^+$
		H_3O^+	2.80E-09	*hydrated*	127	$C_7H_9O^+.H_2O$
		NO^+	2.20E-09	100	108	$C_7H_8O^+$
		O_2^+	2.20E-09	100	108	$C_7H_8O^+$
1-hydroxy-4-ethylbenzene	$C_8H_{10}O$	H_3O^+	2.80E-09	100	123	$C_8H_{11}O^+$
		H_3O^+	2.80E-09	*hydrated*	141	$C_8H_{11}O^+.H_2O$
		NO^+	2.40E-09	100	122	$C_8H_{10}O^+$
		O_2^+	2.40E-09	60	107	$C_7H_7O^+$
		O_2^+	2.40E-09	40	122	$C_8H_{10}O^+$
Decane	$C_{10}H_{22}$	H_3O^+	1.60E-09	100	161	$H_3O^+.C_{10}H_{22}$
		NO^+	1.50E-09	90	141	$C_{10}H_{21}^+$
		O_2^+	2.00E-09	35	142	$C_{10}H_{22}^+$
Dodecane	$C_{12}H_{26}$	H_3O^+	2.80E-09	100	189	$H_3O^+.C_{12}H_{26}$
		NO^+	1.50E-09	90	169	$C_{12}H_{25}^+$
		O_2^+	1.50E-09	40	170	$C_{12}H_{26}^+$

Method 4: SHORT CHAIN FATTY ACIDS						
Compound		Reagent Ion	Reaction Rate	Branching Ratio	Product Ion	
Acetone	C_3H_6O	H_3O^+	3.90E-09	100	59	$C_3H_7O^+$
		H_3O^+	3.90E-09	*hydrated*	77	$(CH_3)2CO.H^+.H_2O$
		NO^+	1.20E-09	100	88	$NO^+.C_3H_6O$
Acetic Acid	CH_3COOH	H_3O^+	2.60E-09	100	61	$CH_3COOH_2^+$
		H_3O^+	2.60E-09	*hydrated*	79	$CH_3COOH_2.H_2O$
		NO^+	9.00E-10	100	90	$NO^+.CH_3COOH$
Propanoic Acid	$C_3H_6O_2$	H_3O^+	2.70E-09	90	75	$C_2H_5COOH_2^+$
		H_3O^+	2.70E-09	*hydrated*	93	$C_2H_5COOH_2^+.H_2O$
		NO^+	1.50E-09	70	104	$NO^+.C_2H_5COOH$
		O_2^+	2.20E-09	80	74	$C_2H_5COOH^+$
Butyric Acid	$C_4H_8O_2$	NO^+	2.40E-09	20	71	$C_3H_7CO^+$
		NO^+	2.40E-09	80	118	$NO^+.C_3H_7COOH$
Pentanoic Acid	$C_5H_{10}O_2$	H_3O^+	2.90E-09	90	103	$C_4H_9COOH_2^+$
		H_3O^+	2.90E-09	*hydrated*	121	$C_4H_9COOH_2^+.H_2O$
		NO^+	2.40E-09	60	85	$C_4H_9CO^+$
		NO^+	2.40E-09	40	132	$NO^+.C_4H_9COOH$
Hexanoic Acid	$C_6H_{12}O_2$	H_3O^+	3.00E-09	25	99	$C_6H_{11}O^+$
		H_3O^+	3.00E-09	75	117	$C_6H_{12}O_2.H^+$
		NO^+	2.50E-09	90	146	$C_6H_{12}O_2.NO^+$

Supplementary Table 2. Example of a spreadsheet containing raw data. The data reported in this table were obtained for the clinical study of Markar et al. in which selected compounds were analysed off-line in breath using SIFT-MS. As a quality control, acetone and humidity have been monitored.

Patient_ID	Humidity (%)	Acetone	Propanoic acid	Butyric acid	Pentanoic acid	Hexanoic acid	Propanal	Butanal	Pentanal	Hexanal	Heptanal	Octanal	Nonanal	Decanal
Patient_1	5.91	1349.4	1.9	50.0	18.0	19.1	23.6	8.4	5.0	2.3	9.8	5.2	4.6	<LOD
Patient_2	5.82	625.7	58.5	48.3	11.7	20.7	23.8	<LOD	12.3	4.3	5.2	4.7	1.2	3.3
Patient_3	5.43	370.7	12.9	51.5	19.6	31.9	21.7	1.0	6.8	11.6	2.8	6.2	4.6	1.8
Patient_4	6.04	906.1	24.3	28.5	10.6	5.1	16.0	1.5	4.5	9.1	8.2	2.7	<LOD	<LOD
Patient_5	5.57	409.6	12.6	21.1	7.2	5.2	6.2	1.1	6.0	2.7	4.4	3.0	4.0	<LOD
Patient_6	5.84	213.5	27.8	82.7	18.8	10.5	45.1	3.6	25.2	5.5	15.0	8.4	8.4	5.2
Patient_7	5.92	639.4	21.5	48.7	10.8	6.4	16.2	4.7	3.0	2.7	11.2	3.4	1.1	<LOD
Patient_8	5.81	562.6	43.4	51.4	14.2	16.5	11.4	7.3	1.2	8.0	6.5	2.9	2.2	3.5
Patient_9	5.38	336.7	40.0	81.3	93.2	26.6	46.0	14.2	187.5	44.0	14.8	8.4	15.7	18.1
Patient_10	5.31	507.0	31.7	45.1	10.3	5.0	8.1	3.2	<LOD	3.3	5.3	1.3	<LOD	1.1
Patient_11	5.36	433.3	10.6	57.4	11.6	8.5	7.6	2.3	1.7	3.2	<LOD	<LOD	4.0	<LOD
Patient_12	5.30	489.7	28.4	63.9	18.3	4.8	12.3	4.6	<LOD	6.1	<LOD	1.9	3.8	1.1
Patient_13	5.51	404.5	24.0	54.4	6.8	13.5	17.4	2.0	7.6	9.2	4.0	<LOD	4.6	1.1
Patient_14	5.54	625.5	1.4	74.9	31.4	19.2	23.1	4.6	9.0	10.4	6.0	3.5	4.1	2.6
Patient_15	5.24	469.7	69.2	94.2	19.9	11.4	46.4	8.3	12.7	6.3	8.4	5.5	3.2	4.4
Patient_16	5.56	2685.7	18.1	93.3	6.3	11.6	35.0	<LOD	1.5	3.9	8.1	1.1	<LOD	<LOD
Patient_17	5.65	1549.2	36.2	54.0	10.1	14.6	23.2	6.6	5.0	3.3	4.6	6.2	2.5	2.9
Patient_18	5.90	370.8	46.2	34.1	8.8	18.3	32.6	3.4	12.8	17.2	4.0	1.6	<LOD	14.6
Patient_19	5.70	248.4	11.7	60.6	12.0	12.5	18.1	1.0	10.9	6.7	6.2	1.8	4.8	2.7
Patient_20	5.82	1576.6	22.4	76.1	7.5	10.7	20.1	3.7	1.2	8.7	2.8	2.7	2.7	2.3
Patient_21	5.59	974.7	65.9	36.7	9.3	26.7	34.5	2.9	4.2	13.4	4.2	1.1	2.6	10.1
Patient_22	5.96	2396.3	26.7	319.7	9.6	10.9	9.7	<LOD	5.0	<LOD	1.9	5.7	3.5	1.3
Patient_23	5.77	410.0	75.5	55.3	17.4	16.8	30.6	2.3	9.0	12.1	14.0	5.9	6.0	6.1
Patient_24	5.84	1164.8	65.5	36.4	9.7	3.3	18.1	<LOD	9.1	4.8	8.5	7.7	6.7	14.0
Patient_25	5.42	505.7	8.4	46.0	8.3	10.2	29.0	3.8	4.2	7.0	6.5	2.7	1.6	3.1

All VOC data are expressed in ppbv, LOD: limit of detection.